High-Performance
Computing Center
Stuttgart

Building a Framework for Effective Data Management with HPC: Strategy and Case studies

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[1] *HLRS High Performance Computing Center Stuttgart*

Workshop on Research Data Management for Data from HPC
15.04.2024

Overview

- HLRS Introduction
- System at HLRS
- Current challenges in RDM
- Use cases
  - NFDI4Cat and Ontology shaped RDM System
  - HLRS Handle server
- Outlook

HLRS

High Performance Computing Center Stuttgart

HLRS Introduction

H L R S

• Since 1960 High Performance Computing • 1982 First German Cray System • 1986 Co-Financing of a Cray by Porsche	University Level
– 1995 First NEC System (SX-4) – 1995 Foundation of HWW for co-operation with industry – 1996 First German Federal HPC center	Federal Center and PPP for Industrial Usage
• 1999 NSF/USA Award • 1999 Initiated European Grid pilot project • 2003 Winner of HPC Challenge at SC'03 • 2004 First TFLOP (NEC SX-8)	Growing Science & Education
– 2007 Co-Founder of **Gauss Center for Supercomputer (GCS)** – 2010 ITEA Gold Award for project ParMA – 2011 First PFLOP (Cray XE6) – 2012 European provider for **PRACE** – 2015 Fastest European System HPCG benchmark (#8 TOP500) – 2018 Project lead for European Center of Excellence in Engineering	European Level

HPC System

Flagship System HPE Apollo System HAWK

- 720.896 cores AMD Rome 64, 2,25 GHz
- Racks: 44
- Nodes: 5.632
- ~26 PetaFlops Peak
- Total Memory: ~1,44 PB
- Infiniband HDR Interconnect (9D Partitial Extended Hypercube Network)
- Pre- and Postprocessing Nodes
- Average Power Consumption: ~3.2 MW

HPC System 2025 - HUNTER

HPC Stepping Stone System

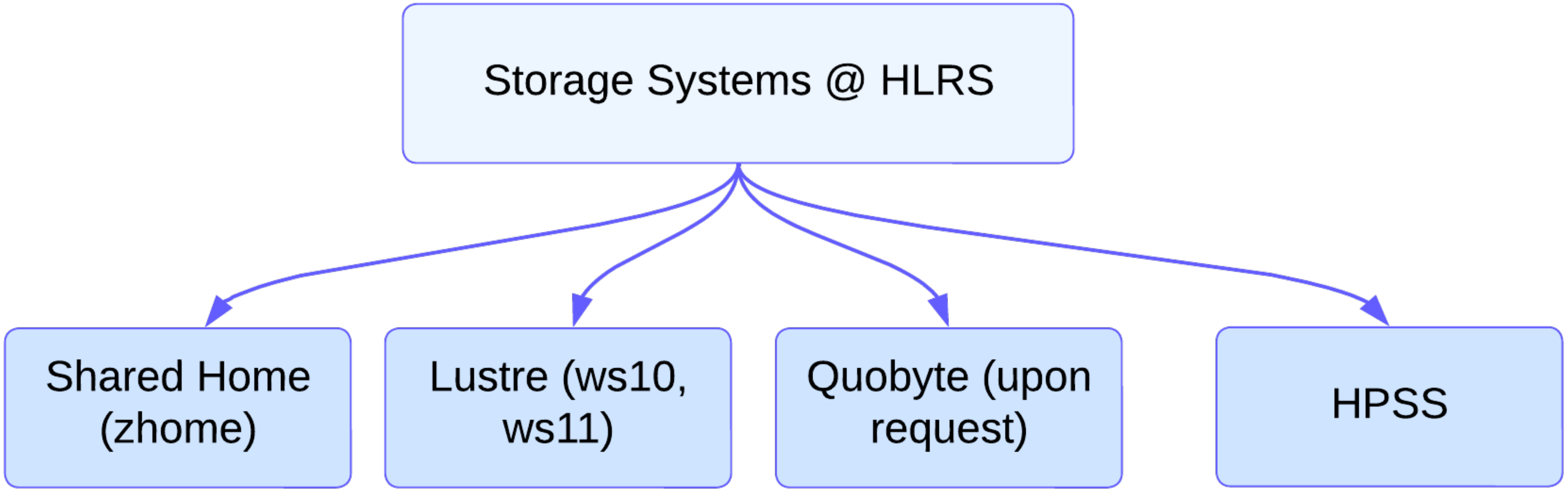
- 544 sockets AMD MI300A (APU)
  - 24 cores and 228 CDNA3 Compute Units
- 136 nodes
- Slingshot Interconnect (4x200 Gbit per node)

- Pre- and Postprocessing Nodes

- Work File Systems
  - HPE Cray ClusterStor E2000 Lustre Appliance
  - FS1: 13PB
  - FS2: 13PB

- Home File System: 540TB

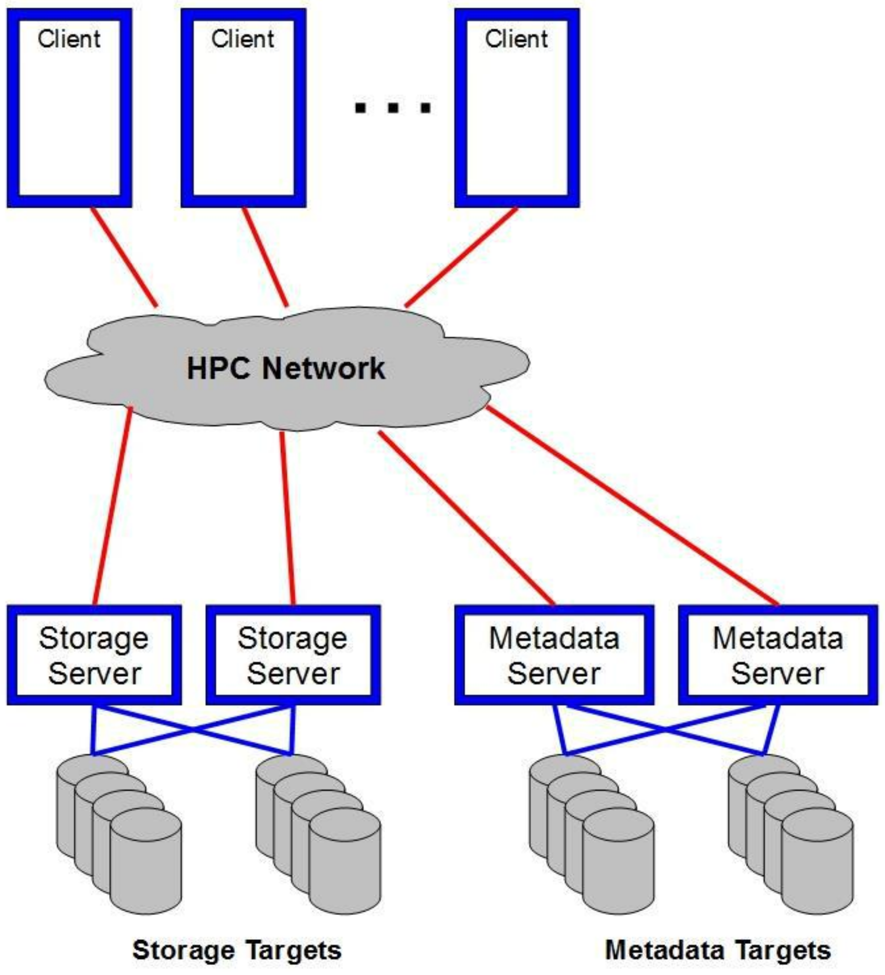
Storage facilities



- Project data
- Scratch data

- Mainly for the projects which require large file counts

Lustre: Asymmetric Parallel Clustered File System



- Sufficient Number of Servers for high throughput
- Sufficient number of disks for high throughput and high capacity
- Manages access of different nodes to the same storage devices (parallel access)
- Organizes concurrent access
- Guarantees data and metadata consistency

Pros.:
- ✓ Scalable Bandwidth
- ✓ Serving high number of clients

Cons.:
- ✗ Metadata Performance
- ✗ sometimes troublesome

Work Space Mechanism

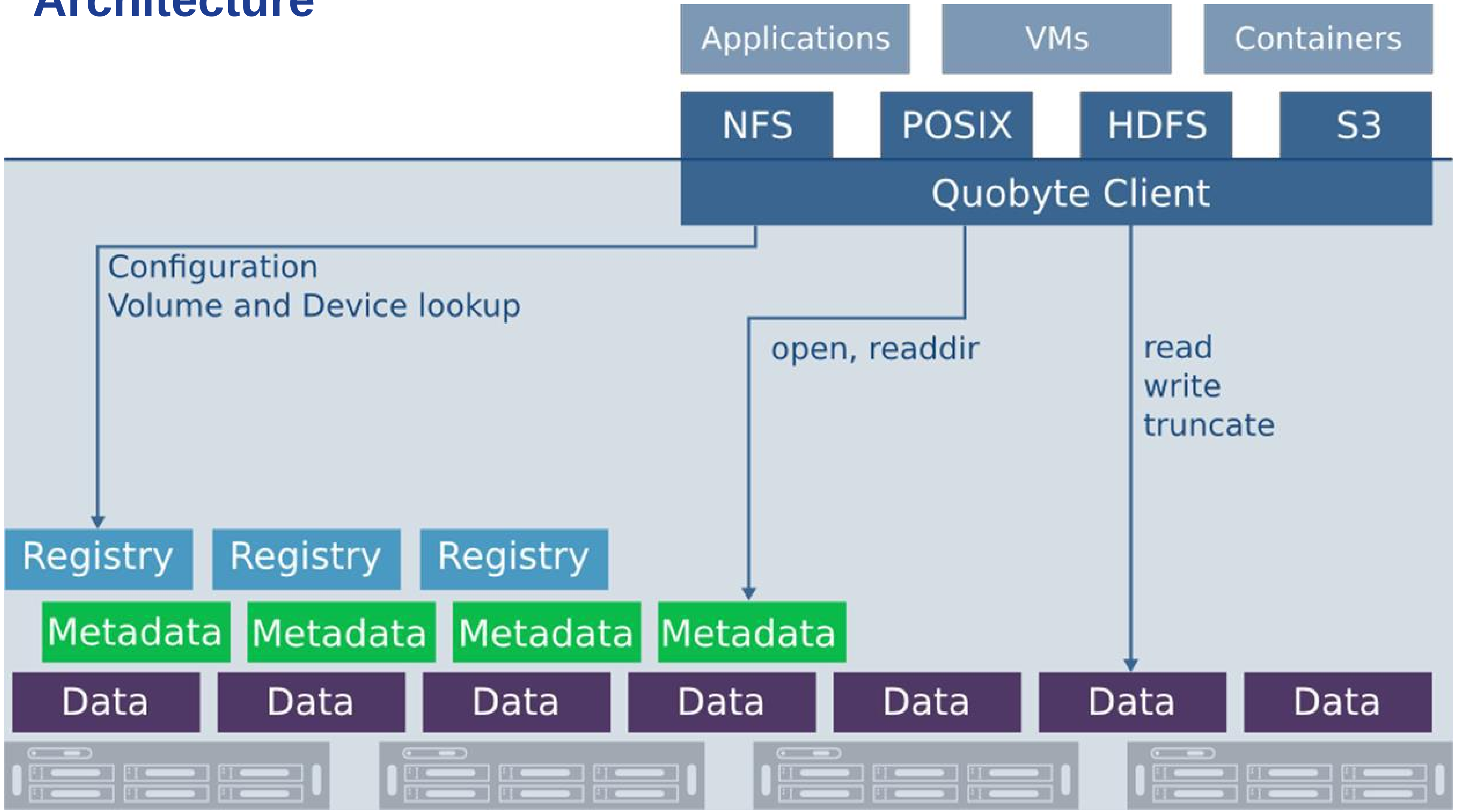
- A directory in the project file system is created upon request with a user defined name;
- The directory is available for 60 days;
- The directory life time can be extended 3 times by 60 days;
- At the end of life, the directory **with its content!!!** is automatically deleted;
- There are tools for:
  - Finding available workspaces;
  - Releasing workspaces;
  - Setting a reminder in calender tools.
- Quota is enabled.

Quobyte - ObjectStore

HLRS

- **Based on Quobyte Data Center File System**
  - Storage as a Service Technology
  - Software-Only-Solution
    - builds a horizontal storage infrastructure from heterogeneous server hardware;
    - avoids vendor lock-in.
- **Goal**
  - Provide Storage Space for special requirements
    - Requirements not feasible for Lustre
  - File System Access to the outside (to come)
  - Other special requirements

Architecture

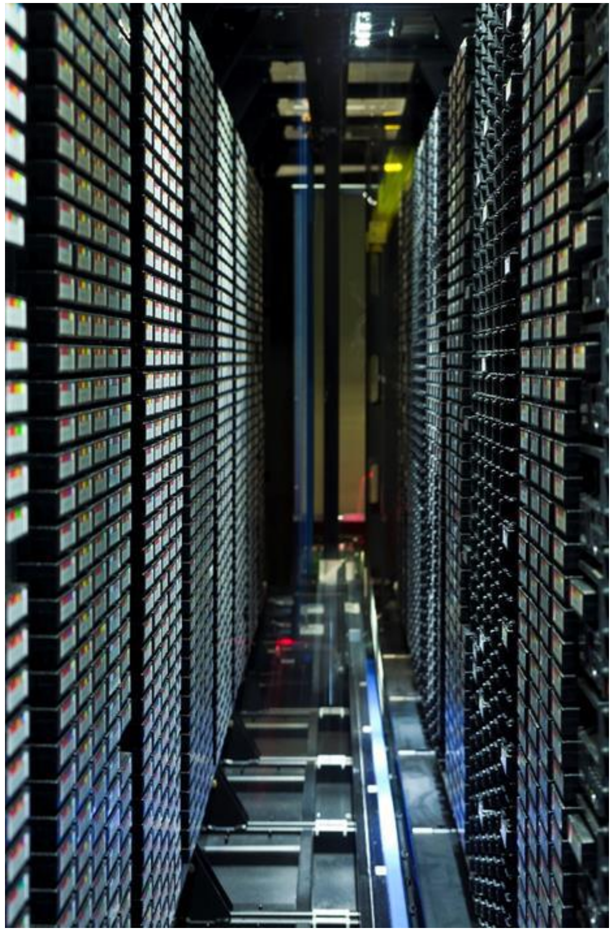


HLRS Installation

- 20 storage units
  - One server
    - 128 GB RAM
    - 2x25 Gbit network connectivity
  - One JBOD
    - 60*10 TB gross capacity each
- 400 Gbit connectivity
- ~12 PB total raw capacity
  - Usable capacity depends on the redundancy schemes in use
- Directly accessible from all Hawk nodes

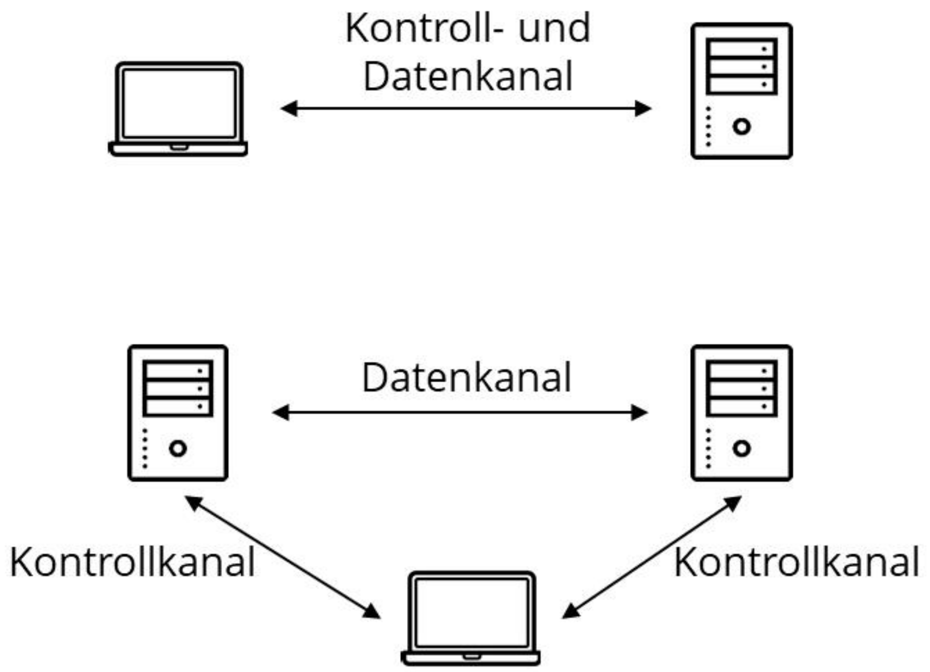
HSM at HLRS (and Backup of Stuttgart University)

- Data Backend using tape technology
- Using HPSS software
- Two copies per file
- Redundant setup



Data Transfer Using GridFTP

- Data Transfer Software developed by Globus project
- Software Stack maintained by Grid CommunityForum
- Features:
    - Acess via certificates
    - Split Setup (frontend/backend) for improved security
    - Features for high speed data transfer like
        - Parallel data connections
        - Parallel data streams



Research Data Management for HPC and current challenges

Current challenges in RDM

HLRS

Data Organization and Structure:
- ✓ Standardized data organization/Metadata standards.

Data Quality and Integrity:
- ✓ Protocols for data/metadata validation/Reproducibility of data.

Data Security and Privacy:
- ✓ Data security measures and standards.

Data Preservation and Longevity:
- ✓ Planning for long-term data preservation.
- ✓

Data Sharing and Collaboration:
- ✓ Data sharing policies and infrastructure.

+ HPC-related:

Data Transfer and Storage:
- ✓ Managing large volumes of data.
- ✓

Data Processing and Analysis:
- ✓ Developing efficient algorithms;
- ✓ Optimizing code.

Resource Allocation and Scheduling:
- ✓ Balancing compute and storage resources.

Performance Monitoring and Optimization:
- ✓ Monitoring system performance

Case studies

NFDI4Cat: Building RDM system for catalysis

- NFDI4Cat – National project for digitalization of catalysis-related sciences.
- Challenges of working with HPC data within catalysis.
- Ontology/**Metadata** as instrument.

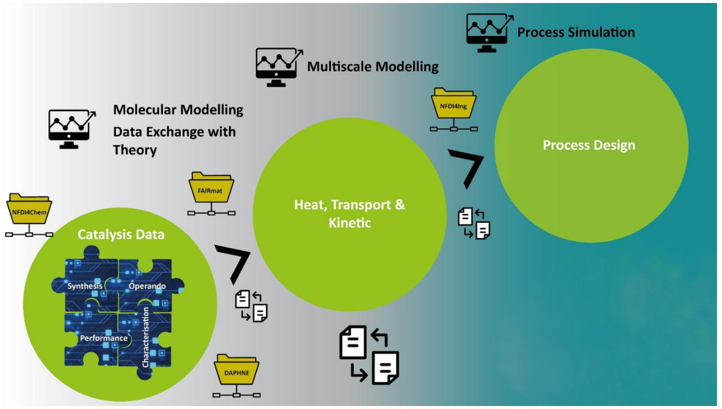


Figure 1. *Multi-Scale Perspectives in Catalysis: From Atomic to Macroscopic Scales, adapted from [1].*

Ontology is a formal specification, which describes the concepts and relationships within a particular domain of knowledge or information.

- poor metadata/ mostly obligatory;
- no understanding of datasets;
- no standards for metadata;
- absence of a user-friendly software for the metadata collection and representation.

[1] Horsch, M. T., Petrenko, T., Schembera, B., & Wentzel, B. (n.d.). Interoperability and architecture requirements analysis and metadata standardization for a research data infrastructure in catalysis. https://www.researchgate.net/publication/352384807

RDM system and approach for metadata enrichment

H L R S

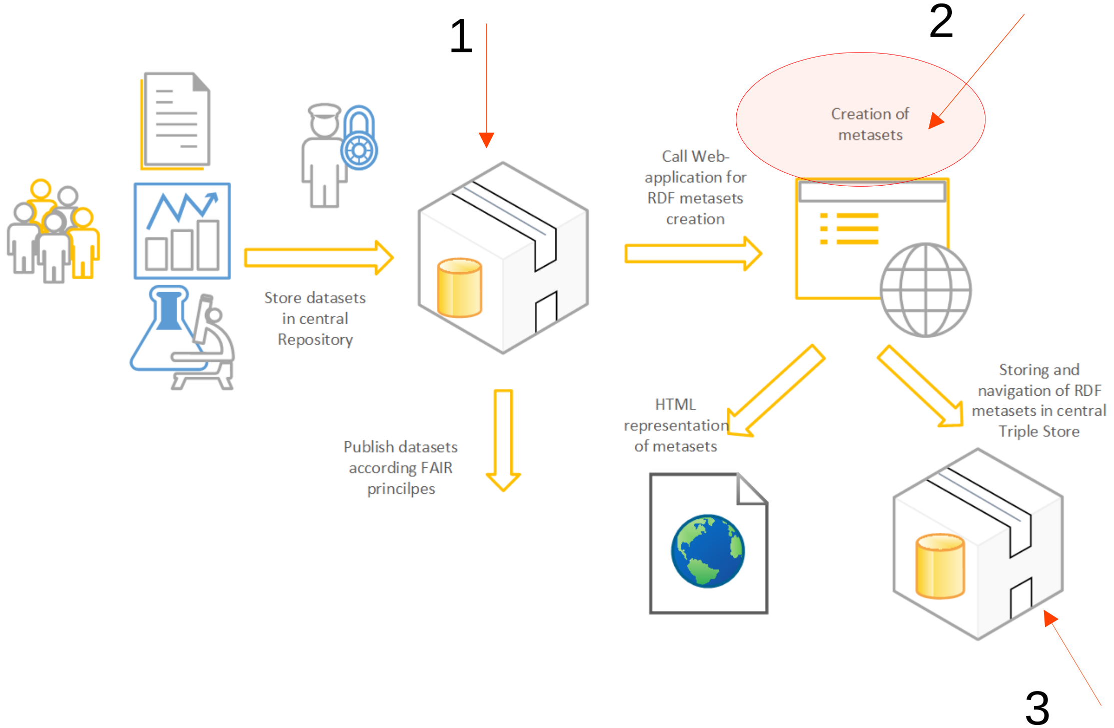
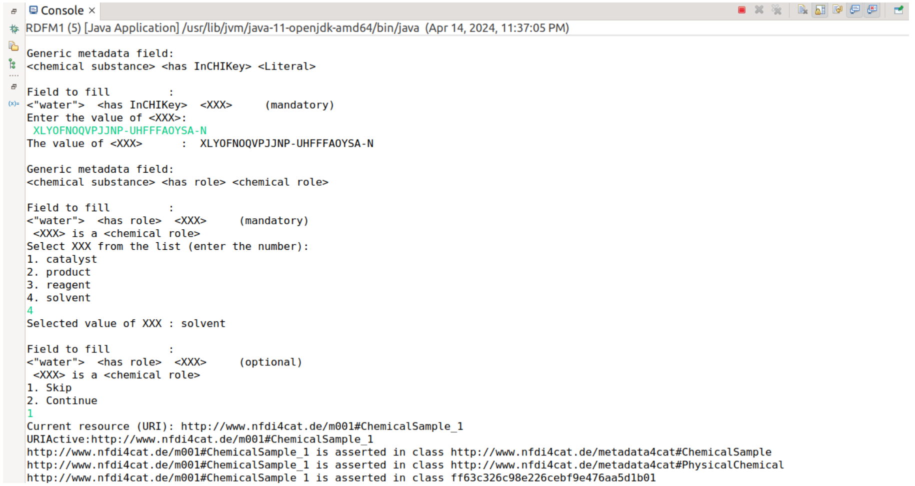


Figure 2. *Schematic representation of RDM system, adapted from [2].*

- **Central Repository**
- **Web-application for the metadata enrichment**
- **RDF database**

- a user-friendly collection of required metadata with connection to the Ontology;
- extending the Metadata4Ing ontology [3] ;
- application of a Use Case-driven approach.



```
Console ×
RDFM1 (5) [Java Application] /usr/lib/jvm/java-11-openjdk-amd64/bin/java  (Apr 14, 2024, 11:37:05 PM)

Generic metadata field:
<chemical substance> <has InCHIKey> <Literal>

Field to fill         :
<"water">  <has InCHIKey>  <XXX>     (mandatory)
Enter the value of <XXX>:
 XLYOFNOQVPJJNP-UHFFFAOYSA-N
The value of <XXX>      :  XLYOFNOQVPJJNP-UHFFFAOYSA-N

Generic metadata field:
<chemical substance> <has role> <chemical role>

Field to fill         :
<"water">  <has role>  <XXX>     (mandatory)
 <XXX> is a <chemical role>
Select XXX from the list (enter the number):
1. catalyst
2. product
3. reagent
4. solvent
4
Selected value of XXX : solvent

Field to fill         :
<"water">  <has role>  <XXX>     (optional)
 <XXX> is a <chemical role>
1. Skip
2. Continue
1
Current resource (URI): http://www.nfdi4cat.de/m001#ChemicalSample_1
URIActive:http://www.nfdi4cat.de/m001#ChemicalSample_1
http://www.nfdi4cat.de/m001#ChemicalSample_1 is asserted in class http://www.nfdi4cat.de/metadata4cat#ChemicalSample
http://www.nfdi4cat.de/m001#ChemicalSample_1 is asserted in class http://www.nfdi4cat.de/metadata4cat#PhysicalChemical
http://www.nfdi4cat.de/m001#ChemicalSample_1 is asserted in class ff63c326c98e226cebf9e476aa5d1b01
```

Figure 3. *Command line realization of the* questionnaire software

[2] 10.5281/zenodo.10964471
[3] https://nfdi4cat.org. (n.d.). Retrieved February 19, 2024, from https://nfdi4cat.org/

Ontology-shaped RDM system

+ Understanding of diverse datasets/ connection to the relevant vocabularies and metadata/data standards.

+ Performing easy search and retrieval, improving efficiency in discovering relevant information.

+ Possibility of the efficient knowledge sharing across projects and disciplines.

+ Simplification of Data Publication process.

? Complexity: can be time-consuming

? Requires training and community support/programming knowledge

? Currently, tool and platform dependencies/ versioning and maintenance

HLRS Handle service

- Prototype of the Service is developed for NFDI4Cat project/application is beyond.
- Support for the creation and management of PIDs.
- Schema can be adjusted.

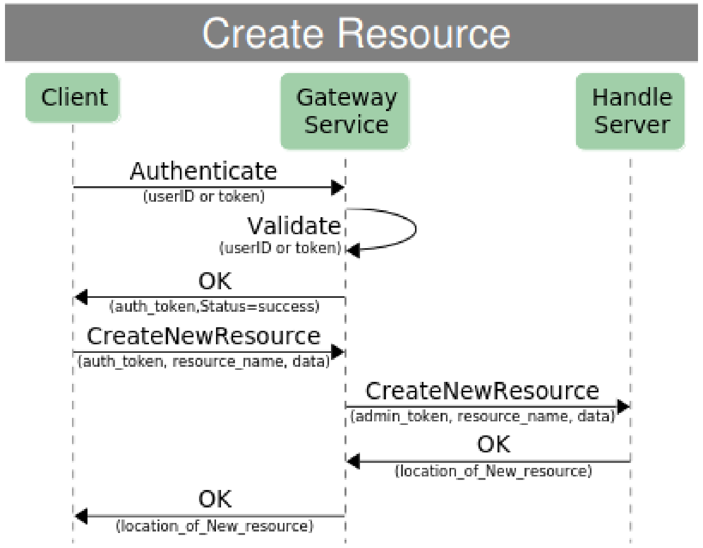


Figure 4. *Schematic representation of HLRS Handle service.*

Why to use?

- Offer more flexibility;
- may provide finer granularity in identifying different aspects or versions;
- supporting multiple identifier schemes.

Outlook

- Collaboration within Community
- Integration with NFDI
- Academia and Industry Collaboration
- Attention to Standards
- Implementation of Real Use-Cases
- Training and Education

Thanks for your attention!

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